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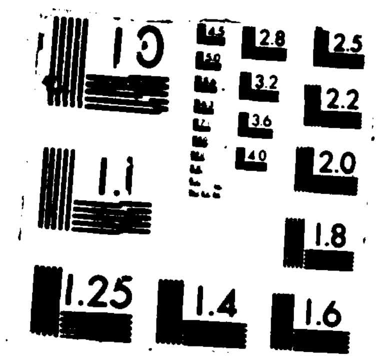

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Sum Rules for Optical Extinction and Scattering by Small Particles

Final Report

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Abstract of First Year Effort

A central problem in developing effective smoke obscurants for space applications is to maximize volumetric extinction or absorption at the wavelength of the incident electromagnetic radiation. Although this is a problem without a general solution, it is possible to make recommendations based on very general considerations. One can establish bounds not on extinction at any wavelength, but rather extinction integrated over all wavelengths.

A sum rule for extinction is a bound on integrated volumetric extinction. The existence of such sum rules requires suitable behavior of volumetric extinction at high and low frequencies. If, in the limit of low frequency, extinction decreases as the $1 + \sigma$ power of frequency, where σ is any positive number, then a sum rule exists. At low frequencies, the extinction cross section of an ellipsoid composed of either a simple free-electron metal or a simple insulator is proportional to frequency squared, which ensures the existence of a sum rule for extinction by such particles. Only a single type of sum rule exists because of the rather stringent requirements on both the low- and high-frequency behavior of particle extinction cross sections.

We have established that the sum rule for extinction is not changed when magnetic dipole as well as electric dipole radiation is considered. Moreover, the limitation of electron mean free paths in metallic particles does not invalidate sum

rules. When metallic particles are sufficiently small, the effect of their boundaries is to decrease peak extinction while simultaneously broadening it in such a way that integrated extinction remains constant.

Although integrated extinction is independent of particle size, sum rules imply that the smallest particles will have the greatest volumetric extinction. When a particle is illuminated by an electromagnetic wave, various electromagnetic modes are excited. The larger the particle, the greater the number of modes. Thus, a fixed amount of total extinction must be shared by modes, the number of which increases with increasing particle size. This implies that the smallest particles have the greatest extinction.

Two classes of materials, free-electron metals and polar insulators, with vastly different properties, nevertheless have in common that integrated extinction by particles of these materials is approximately the same.

Volumetric extinction of 10^4 cm^{-1} should be looked upon as a kind of lower bound: it is the value that can be obtained without much effort. What is the upper bound? We must look to small (compared with the wavelength) metallic particles for the greatest possible volumetric extinction. Fewer modes are excited in a sphere than in a needle or a disk. Peak extinction by a small aluminum sphere is about 10^7 cm^{-1}. We claim that this is a practical upper bound. Moreover, this bound cannot be obtained over a wide range of frequencies. A practical upper bound over at least one decade from the ultraviolet to the near infrared is 10^6 cm^{-1}, and this would have to be obtained with a mixture of particles having different shapes.

Abstract of Second Year Effort

One of the essential lessons to be learned from sum rules is that extinction cannot be arbitrarily specified. Integrated volumetric extinction is independent of particle size and depends on only the low frequency behavior of the material of which the particle is composed. This in turn implies that extinction at one frequency is related to extinction at other frequencies. From this idea another related one evolved: the scattering coefficients are not independent. A proof of this was constructed for scattering by a sphere. The Mie coefficients are completely specified by the first four of them. A proof of this and its physical interpretation is given in Appendix A, a manuscript on recurrence relations for Mie scattering coefficients, which will appear in a future issue of Journal of the Optical Society of America.

Appendix A

Recurrence Relations for the Mie Scattering Coefficients

to appear in

<u>Journal</u> <u>of</u> <u>the</u> <u>Optical</u> <u>Society</u> <u>of</u> <u>America</u>

February 1987

Recurrence Relations for the Mie Scattering Coefficients

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Abstract

The Mie scattering coefficients satisfy recurrence relations: a_{n-1}, b_{n-1}, a_n, and b_n, determine a_{n+1} and b_{n+1}. It is therefore possible, in principle, to generate the entire set from the first four, which has a simple interpretation. Each term in a multipole expansion of an electrostatic field can be obtained by differentiating the preceding term. The Mie coefficients are terms in a multipole expansion of a particular electromagnetic field, that scattered by an arbitrary sphere. By analogy, it is not surprising that all these coefficients can be generated from the electric and magnetic dipole and quadrupole terms. Moreover, the recurrence relations for the Mie coefficients contain finite differences, in analogy with the infinitesimal differences (derivatives) in the multipole expansion of an electrostatic field.

The solution to the problem of scattering by an arbitrary sphere (Mie theory) yields an infinite set of coefficients[1-5], which depend on various Bessel functions and their derivatives. The usual approach to computing these coefficients is to compute the Bessel functions by recurrence[5-8]. This might be called the natural or direct way of computation. It seems so natural, so obvious, that, to my knowledge, no one has ever done otherwise, although there are hints in Ref. 4 (p. 51). What is usually at issue is not <u>if</u> one should compute Bessel functions but rather <u>how</u> to do it in the fastest and most accurate way. I have posed this question differently. The Bessel functions in the expressions for the scattering coefficients satisfy recurrence relations. Furthermore, Verner[9] showed that the numerators and denominators of these coefficients satisfy recurrence relations. Thus, is it not likely that the coefficients themselves satisfy recurrence relations? In the following paragraphs I show that they do and give a physical interpretation of why. My notation and conventions are those of Ref. 5.

The Mie scattering coefficients can be written as follows:

$$a_n = \frac{xD_n(mx)\psi_n(x) + mn\psi_n(x) - mx\psi_{n-1}(x)}{xD_n(mx)\xi_n(x) + mn\xi_n(x) - mx\xi_{n-1}(x)}, \tag{1}$$

$$b_n = \frac{mxD_n(mx)\psi_n(x) + n\psi_n(x) - x\psi_{n-1}(x)}{mxD_n(mx)\xi_n(x) + n\xi_n(x) - x\xi_{n-1}(x)}, \tag{2}$$

where D_n is the logarithmic derivative ψ_n'/ψ_n, and ψ_n, ξ_n are Riccati-Bessel functions. The size parameter x is $2\pi a/\lambda$, where a is the radius of the sphere and λ is the wavelength of the incident light; m is the refractive index of the sphere relative to that of the surrounding medium. The logarithmic derivative satisfies the recurrence relation

$$D_{n-1} = \frac{n}{mx} - \frac{1}{D_n + n/mx} , \qquad (3)$$

and both of the Riccati-Bessel functions satisfy the recurrence relation

$$z_{n-1} = \frac{2n + 1}{x} z_n - z_{n+1} . \qquad (4)$$

From Eqs. (1)-(4) it follows that any set of six coefficients are given by

$$a_{n-1} = \frac{uy + A_3uz + B_1y + A_4z}{uv + A_3uw + B_1v + A_4w} , \qquad (5)$$

$$b_{n-1} = \frac{uy + B_1y + A_2z}{uv + B_1v + A_2w} , \qquad (6)$$

$$a_n = \frac{uy + A_1y + A_2z}{uv + A_1v + A_2w} \qquad (7)$$

$$b_n = \frac{uy + B_1y + B_2z}{uv + B_1v + B_2w} , \qquad (8)$$

$$a_{n+1} = \frac{uy + A_5uz + A_6y + A_7z}{uv + A_5uw + A_6v + A_7w} , \qquad (9)$$

$$b_{n+1} = \frac{uy + [illegible] + A_2z}{uv + [illegible] + A_2w} , \qquad (10)$$

where $u = D_n$, $v = \xi_n$, $w = $ [illegible]$_{n-1}$, $y = \psi_n$, $z = \psi_{n-1}$ and

$$A_1 = \frac{mn}{x}, \quad A_2 = -m, \quad B_1 = \frac{n}{mx}, \quad B_2 = -1/m,$$

$$A_3 = \frac{n(1 - m^2)}{m^2 x}, \quad A_4 = \frac{n^2 - m^2x^2 - m^2n^2}{m^3x^2},$$

$$A_5 = \frac{x(m^2 - 1)(n + 1)}{(n + 1)(2n + 1)(1 - m^2) + m^2x^2},$$

$$A_6 = \frac{nm^2x + (n + 1)^2(2n + 1)(m^2 - 1)}{mx\{(n + 1)(2n + 1)(1 - m^2) + m^2x^2\}},$$

$$A_7 = \frac{(n + 1)^2(1 - m^2) - m^2x^2}{m\{(n + 1)(2n + 1)(1 - m^2) + m^2x^2\}},$$

$$B_3 = \frac{(2n + 1)m^2 - (n + 1)}{mx}.$$

Four quantities (e.g., u, v/y, w/y, z/y) determine any of the five coefficients a_{n-1}, b_{n-1}, a_n, b_n, a_{n+1} (or b_{n+1}). Thus, it is possible to solve for any one of these coefficients (e.g., a_{n+1} or b_{n+1}) in terms of the other four. To do so, we may consider u to be fixed in Eqs. (5)-(8) and write them in the form

$$\begin{pmatrix} a_n(A_1 + u) & a_nA_2 & -(A_1 + u) & -A_2 \\ b_n(B_1 + u) & b_nB_2 & -(B_1 + u) & -B_2 \\ b_{n-1}(B_1 + u) & b_{n-1}A_2 & -(B_1 + u) & -A_2 \\ a_{n-1}(B_1 + u) & a_{n-1}(A_3u + A_4) & -(B_1 + u) & -(A_3u + A_4) \end{pmatrix} \begin{pmatrix} v \\ w \\ y \\ z \end{pmatrix} = 0 \qquad (11)$$

The determinant of the coefficient matrix in Eq. (11) must vanish if its solution is to be nontrivial. By setting this determinant equal to zero, one obtains a cubic equation satisfied by u. One of its factors is $B_1 + u$, which follows from inspection of Eq. (11); the root $u = -B_1$ is obviously not the one desired. The correct value of u is one of the roots of the quadratic equation

$$u^2 - \left(A_1\Delta + \frac{A_2 - A_4}{A_3}\right)u + \frac{A_1(B_2 - A_4)}{A_3}\,\Delta = 0, \qquad (12)$$

where

$$\Delta = \frac{(a_n - b_n)(a_{n-1} - b_{n-1})}{(b_n - a_{n-1})(a_n - b_{n-1})} \; . \qquad (13)$$

To obtain these equations it was also necessary to use the relations $A_2B_2 = 1$ and $A_1B_2 = A_2B_1$. Which of the two roots of Eq. (12) is the correct one must be determined by some auxiliary condition (e.g., the magnitude of the scattering coefficients cannot exceed unity). Given this root, one can substitute it in Eq. (11) and determine any three of the set (v,w,y,z) as multiplicative functions of the fourth. When these functions and u are substituted into Eq. (9), a_{n+1} is obtained as a function of a_{n-1}, b_{n-1}, a_n, b_n, the index n, and the properties of the sphere (x and m). Similarly, b_{n+1} is so obtained. This completes the proof that any set of four consecutive scattering coefficients determine the following two.

This result has a simple interpretation. It has long been known that each term in the expansion of an electrostatic field can be obtained by differentiation of the preceding term. This idea was developed by Maxwell[10,11], who used the term "points" of the nth order, whereas in modern work they would be referred to as "2^n poles" or "multipoles" (see, e.g., Ref. 12). The Mie coefficients are terms in a multipole expansion of a particular electromagnetic field, that scattered by an arbitrary sphere. By analogy, it is not surprising that all of these coefficients can be generated from the electric (a_1) and magnetic (b_1) dipole terms and the electric (a_2) and magnetic (b_2) quadrupole terms. Moreover, the recurrence relations for the Mie coefficients contain finite differences (see Eq. 13), in analogy with the infinitesimal differences (derivatives) in the multipole expansion of an electrostatic field. A possible interpretation of why the multipoles in Mie theory are connected by finite differences is that this theory applies to particles with finite (relative to the wavelength) dimensions. In contrast, the wavelength is infinite (alternatively, the speed of light is infinite) in electrostatics. A further difference between electrostatics (and magnetostatics) and electrodynamics is that in static theories the electric and magnetic terms are distinct: electric terms are connected only to electric terms (and similarly for magnetic terms). But when the propagation time over characteristic distances is not negligible compared with the period (e.g., when $x = \omega a/c$ is not negligible, where c is the speed of light, and a is the radius of a particle illuminated by light of circular frequency ω), then electric and magnetic multipoles are inextricably connected.

Whether or not the recurrence relations can simplify scattering calculations must be determined by extensive calculations. It is not known if the recurrence relations are stable, either upward or downward. And one must devise a simple test for which root of Eq. (12) is the proper one. These are matters for further investigation. Nevertheless, merely knowing that the scattering coefficients can be generated by recurrence gives new insights. It is for this reason that I have set them down, not because they will necessarily reduce computation time.

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References

1. J. A. Stratton, Electromagnetic Theory (McGraw-Hill, New York, 1941), Sec. 9.25.

2. H. C. van de Hulst, Light Scattering by Small Particles (Wiley, New York, 1957), Ch. 9.

3. M. Born and E. Wolf, Principles of Optics, 3rd. ed. (Pergamon, Oxford, 1965), Sec. 13.5.

4. M. Kerker, The Scattering of Light and Other Electromagnetic Radiation (Academic, New York, 1969), Chs. 3 and 4.

5. C. F. Bohren and D. R. Huffman, Absorption and Scattering of Light by Small Particles (Wiley-Interscience, New York, 1983), Ch. 4.

6. J. V. Dave, Subroutines for Computing the Parameters of the Electromagnetic Radiation Scattered by a Sphere, IBM Order Number 360D-17.4.002 (1968).

7. W. J. Lentz, "Generating Bessel functions in Mie scattering calculations using continued fractions," Appl. Opt. 15, 668 (1976).

8. W. J. Wiscombe, "Improved Mie scattering algorithms," Appl. Opt. 19, 1505 (1980).

9. B. Verner, "Note on the recurrence between Mie's coefficients," J. Opt. Soc. Am. 66, 1424 (1976).

10. J. C. Maxwell, A Treatise on Electricity and Magnetism, Vol. 1 (Dover, New York, 1954), p. 196.

11. E. W. Hobson, The Theory of Spherical and Ellipsoidal Harmonics (Cambridge University Press), pp. 129-132.

12. W. K. H. Panofsky and M. Phillips, Classical Electricity and Magnetism (Addison-Wesley, Reading, Mass., 1962), p. 15.

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